

Acetamide, N-methyl-N-phenyl-

Other names:	Acetanilide, N-methyl- Acetomethylanilide Exalgin Methylantifebrin Methylazol N-Acetyl-N-methylaniline N-Acetyl-methylaniline N-Methyl-N-phenylacetamide N-Methylacetanilide NSC 2140 Oxalgin Phenylmethylacetamide
Inchi:	InChI=1S/C9H11NO/c1-8(11)10(2)9-6-4-3-5-7-9/h3-7H,1-2H3
InchiKey:	LMTGCJANOQOGPI-UHFFFAOYSA-N
Formula:	C9H11NO
SMILES:	CC(=O)N(C)c1ccccc1
Mol. weight [g/mol]:	149.19
CAS:	579-10-2

Physical Properties

Property code	Value	Unit	Source
gf	119.17	kJ/mol	Joback Method
hf	-37.61	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	46.69	kJ/mol	Joback Method
ie	8.81	eV	NIST Webbook
log10ws	-0.95		Aqueous Solubility Prediction Method
logp	1.669		Crippen Method
mcpvol	125.460	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1260.00		NIST Webbook
rinpol	1260.00		NIST Webbook
tb	498.31	K	Joback Method
tc	713.50	K	Joback Method
tf	300.01	K	Joback Method
vc	0.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.71	J/mol×K	498.31	Joback Method
cpg	279.54	J/mol×K	534.18	Joback Method
cpg	292.46	J/mol×K	570.04	Joback Method
cpg	304.53	J/mol×K	605.91	Joback Method
cpg	315.77	J/mol×K	641.77	Joback Method
cpg	326.23	J/mol×K	677.64	Joback Method
cpg	335.96	J/mol×K	713.50	Joback Method
hvapt	60.10	kJ/mol	451.00	NIST Webbook
hvapt	56.70	kJ/mol	451.50	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C579102&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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